AN APPROACH FOR MODELING ROCK DISCONTINUOUS BEHAVIOR UNDER MULTIPHASE FLUID FLOW CONDITIONS

Peng-Zhi Pan[1,2], Jonny Rutqvist[2], Fei Yan[1], Xiating Feng[1]

[1]   State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of
Rock and Soil Mechanics, Chinese Academy of Sciences, Wuhan, 430071, China.
[2]   Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
e-mail: ppan@lbl.gov

ABSTRACT

In this paper, we report the integration of two computer codes, TOUGH2 and RDCA (Rock Discontinuous Cellular Automaton), for coupled hydromechanical analysis of multiphase fluid flow and discontinuous behavior in heterogeneous rock. The RDCA is a numerical model being developed for simulating the nonlinear and discontinuous behavior of rock. TOUGH2 is a well-established code for geo-hydrological analysis with multiphase, multicomponent fluid flow and heat transport. The integration of these two codes is executed sequentially and linked through external coupling modules. TOUGH2 modeling provides the changes in effective stress as a function of multiphase pore pressure and thermal expansion. RDCA corrects porosity, permeability, and capillary pressure for changes in mechanical behavior. By introducing discontinuous function in RDCA, we can conveniently apply the fluid pressure obtained from TOUGH2 to any discontinuous inner boundaries. As a result, rock nonlinear and discontinuous deformation behavior, such as plastic yielding, crack initiation, propagation and coalescence etc., induced by the change of fluid pressure and thermal expansion, can be simulated in RDCA. RDCA incorporates the discontinuity of a crack independently of the mesh, such that the crack can be arbitrarily located within an element. The method does not require any re-meshing for crack growth, which greatly simplifies the modeling procedure and its integration with TOUGH2. Here, we provide a detailed description of TOUGH-RDCA integration and then present numerical examples to show the combined code's capability to model discontinuous deformation and fracturing of rock masses within a multiphase fluid flow environment.

INTRODUCTION

Rock masses are generally strongly heterogeneous, containing rock matrix and discontinuities. Rock masses may be exposed to complex environments, such as mechanical, hydraulic, and thermal fields and their couplings. The study of coupled thermal-hydro-mechanical (THM) processes is key for understanding the complex physical behavior within rock masses. In the last few decades, a steadily growing interest in coupled THM phenomena in geological media has encouraged development of many computer codes at various levels of sophistication. Based on Biot's theory of consolidation, several simulators such as THAMES (Ohnishi et al., 1996), MOTIF (Guvanasen and Chan, 1995), FRACON (Nguyen, 1996) and ROCMAS (Noorishad et al. 1984) were developed and applied mostly to geological nuclear waste disposal. Other simulators (FEMH (Bower and Zyvoloski, 1997), GeoSys/Rockflow (Wang and Kolditz, 2007), FRACTure (Kohl and Hopkirk, 1995), GEOCRACK (Swenson et al., 1997)) were originally applied to the field of hot-dry-rock geothermal energy, although they have also been applied to other types of coupled problems. Some commercial codes (e.g., ABAQUS (Börgesson, 1996), FLAC (Israelsson, 1996), UDEC (Israelsson, 1996)) have been applied in soil and rock mechanics. In the field of soil mechanics, COMPASS (Thomas and Sansom, 1995) and CODE-BRIGHT (Olivella et al., 1994) were developed to simulate coupled two-phase (gas and liquid) fluid flow and thermo-mechanical responses in partially saturated soil and isothermal multiphase flow of brine and gas in saline media. TOUGH2, developed by Pruess et al. (1999), is a well established numerical model that can simulate non-isothermal, multiphase flow processes. Because TOUGH2 does not include mechanical modules, a practical way

to consider the mechanical effect is to link it with other codes. Rutqvist and Tsang (2002) and Rutqvist et al. (2002) pioneered this approach by linking TOUGH2 (Pruess et al., 1999) and FLAC3D (Itasca Consulting Group, 2000) for modeling multiphase flow, heat transport and geomechanics.

The codes and numerical methods mentioned above are versatile in modeling coupled THM processes, including some of them under multiphase flow conditions. However, the ability to model nonlinear and discontinuous behavior in rock masses, including fracture propagation, under multiphase flow and non-isothermal conditions, still needs to be strengthened. Rock masses are generally heterogeneous, containing different minerals, joints, and fractures. Under such conditions, the rock mass behavior can be nonlinear and discontinuous, with strong coupling between THM processes. Therefore, we require an appropriate numerical model that can adequately consider the heterogeneous and discontinuous behavior of rock and simulate its fracturing process under strongly coupled THM conditions.

The Rock Discontinuous Cellular Automaton (RDCA) (Pan et al., 2012) code, developed to simulate the fracturing process in heterogeneous rock, is effective in considering the nonlinearity and discontinuity of rocks. RDCA contains a thermo-hydro-mechanical module, but is limited to single-phase fluid flow (Pan et al. 2009). This paper describes taking the RDCA approach a step further by linking TOUGH and RDCA for modeling the nonlinear and discontinuous behavior of heterogeneous rock under multiphase flow and nonisothermal conditions. We present coupling functions and a linking approach, and then show numerical examples demonstrating the capability of the coupled TOUGH-RDCA simulator.

NUMERICAL TOOL—A COMBINATION OF TOUGH-RDCA

An Introduction to the Rock Discontinuous Cellular Automaton (RDCA) Code

The Rock Discontinuous Cellular Automaton (RDCA) (Pan et al., 2012) incorporates the following methods and techniques: (1) a special

displacement function to represent internal discontinuity; (2) a level set method to track the fracturing path; (3) a partition of unity method to improve the integral precision of fracture surface and fracture tip; (4) a cellular automaton updating rule to calculate the mechanical state; (5) a mixed-mode fracture criterion to determine the fracturing behavior. By doing so, this code incorporates the discontinuity of a crack independently of the mesh, such that the crack can be arbitrarily located within an element. The method does not require any re-meshing for crack growth. These aspects greatly reduce the complexity and improve modeling efficiency.

The previous version of RDCA did not include the function for modeling discontinuous deformation behavior induced by fluid injection. To do that, we discretize the domain to be solved into a system of cell elements in which the discontinuity of a crack is incorporated (Figure 1). To extend this approach to fracturing under internal fluid pressure, we also discretize the crack surface into one-dimensional segments used for applying fluid pressure on the two opposing crack surfaces. Gaussian quadrature points are defined along each of the one-dimensional subelements to numerically integrate the terms on Γ_c (Figure 2). Each Gaussian point coordinate on Γ_c is mapped on global coordinates, which are then mapped within the local coordinate system to cell elements. A Gaussian quadrature is performed by a loop over one-dimensional elements. The nodal forces induced by fluid pressure on crack surfaces and crack tips can be respectively calculated as

$$f_i^a = 2\int_{\Gamma_c} \mathbf{n} \cdot N_i \mathbf{p} \, d\Gamma \qquad (1)$$

$$f_i^{b\alpha} = 2\int_{\Gamma_c} \mathbf{n}\sqrt{r} \cdot N_i \mathbf{p} \, d\Gamma \qquad \alpha = 1,2,3,4 \quad (2)$$

where $\mathbf{p}$ is the fluid pressure applied on the crack surfaces. $\mathbf{n}$ is a vector normal to crack surface. r is the radius for integration around the crack tip. Ni is shape function. To judge whether a crack propagates, we introduce linear-elastic-fracture mechanics and the stress intensity factor concept (SIF) (Knott 1973; Broek 1982; Kanninen and Popelar 1985; Atkinson 1987). For a two-dimensional problem, the stress intensity factor for mixed mode failure is

$$J = \frac{K_I^2}{E^*} + \frac{K_{II}^2}{E^*} \qquad (3)$$

For plane stress, $E^* = E$, whereas for plane strain, $E^* = \frac{E}{1-v^2}$.
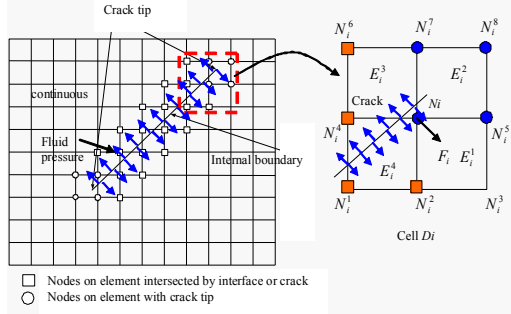

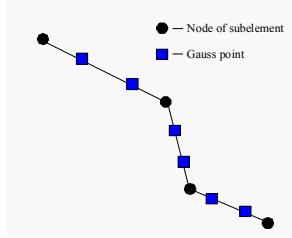Figure 1. Representation of the discontinuous cellular automaton model

Figure 2. Gauss quadrature points on a crack surface.

Consider two equilibrium states of the body, i.e., State 1 and State 2. State 1 is the actual state of the body; State 2 is an auxiliary state. Field variables associated with the two states are denoted with superscripts 1 and 2. Superposition of the two equilibrium states leads to another equilibrium state denoted by $J^{(1+2)}$.

$$J^{(1+2)} = \int_\Gamma \left[\frac{1}{2} \left(\sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} \right) \left(\varepsilon_{ij}^{(1)} + \varepsilon_{ij}^{(2)} \right) \delta_{1j} - \left(\sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} \right) \frac{\partial \left(u_i^{(1)} + u_i^{(2)} \right)}{\partial x_j} \right] n_j \, d\Gamma \qquad (4)$$

We can write a simplified form of the above equation:

$$J^{(1+2)} = J^{(1)} + J^{(2)} + M^{(1,2)} \qquad (5)$$

Assuming that the crack surface near the crack tip is straight and is in the integral boundary C_0 shown in Figure 3, the M-integral can be expressed as,

$$M^{(1,2)} = \int_C \left[\sigma_{ij}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} + \sigma_{ij}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} - W^{(1,2)} \delta_{1j} \right] q m_j \, dC - \qquad (6)$$

$$\int_{C_+ + C_-} \left[\sigma_{i2}^{(1)} \frac{\partial u_i^{(2)}}{\partial x_1} + \sigma_{i2}^{(2)} \frac{\partial u_i^{(1)}}{\partial x_1} - W^{(1,2)} \delta_{1j} \right] q m_j \, dC$$

where $C = \Gamma \cup C_+ \cup C_- \cup C_0$, m_j is the outward normal vector to domain and q is the weight function. The second term of the right-hand side in Eq. (6) considers the effect of fluid pressure on crack surface.
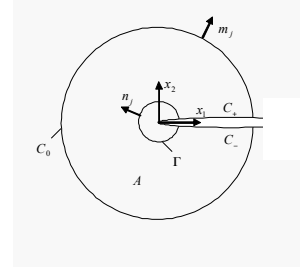

Figure 3. Representation of M-integral at the crack tip

Rock-mass failure can be induced by mixed-mode cracking. In RDCA, several criteria, such as the maximum circumferential stress criterion, maximum tangential stress criterion, and minimum strain energy criterion, are used to determine the cracking conditions. During the simulation, the criterion provides the amount and direction of crack advancement. Take the maximum circumferential stress criterion as an example: an explicit solution for the direction of crack propagation would be:

$$\theta_c = 2 \tan^{-1} \left[\frac{1}{4} \left(\frac{K_I}{K_{II}} - \text{sign}(K_{II}) \sqrt{8 + \left(\frac{K_I}{K_{II}} \right)^2} \right) \right] \qquad (7)$$

where θ_c is measured with respect to a local polar coordinate system with its origin at the crack tip, and is aligned in the direction of the existing crack. Once the crack-growth orientation is determined, a propagation increment is added to the existing crack, and the analysis procedure is repeated. Stress intensity factors K_I and K_{II} are calculated using the domain form of the interaction integral.

An Introduction to TOUGH2
TOUGH2 is a well-established numerical simulation program for multidimensional fluid and heat flows of multiphase, multicomponent fluid mixtures in porous and fractured media. It has been widely used in geothermal reservoir engineering, nuclear waste isolation studies, environmental assessment and remediation, and flow and transport in variably saturated media and

aquifers. Detailed description can be found in the work by Pruess et al. (Pruess et al. 1999; Pruess and Garc¨ªa 2002)

The Combination of TOUGH-RDCA

In this work, the coupled THM analysis is conducted by combining TOUGH2 and RDCA. Figure 4 shows the relation between TOUGH2 and RDCA codes in the THM coupling modeling. A TOUGH-to-RDCA link takes multiphase pressures, saturation and temperature from the TOUGH2 simulation and provides the updated temperature and pore-pressure information to RDCA. In RDCA, the thermal expansion and effective stress is calculated, and then the failure analysis (plasticity or discontinuity) is conducted. An RDCA-to-TOUGH link takes the mechanical variables (stress, plastic strain or fracture opening displacement) from RDCA and updates the corresponding element porosity, permeability, and capillary pressure to be used by TOUGH2.

The combined simulator can model nonisothermal, multiphase flow processes coupled with mechanical behavior changes induced by temperature and fluid pressure. One of the main features of the RDCA mechanical model is the ability to analyze the stress path, nonlinearity, and discontinuity in a rock mass that might be critically stressed, on the verge of failure because of THM effects.

To run a TOUGH-RDCA simulation, the numerical grids for the two codes should be developed with the same geometry and element numbering. In RDCA, the crack geometry (or other internal boundaries) and numerical grid are independent of each other. Using the level-set method, we divide the elements intersected by a crack into several quadrilateral sub-elements based on the *partition of unity* concept (Figure 5). The pressure in each element is determined from the solution of the flow equation over the entire domain. For elements intersected by the crack, the fluid pressure is applied on the crack surface. As seen from Figure 5, the fluid pressure applied on the crack surface can be non-uniform, since different places may have different fluid pressures.

The mechanical response is calculated by the equivalent nodal force induced by fluid pressure.

Based on the fluid pressure on each element, the equivalent nodal force can be calculated using the effective stress theory. For a normal element, i.e., with no crack surface or crack tip included, the equivalent nodal forces can be calculated by

$$\{f\}^e = \int_{\Omega^e} [B]^T \{p, p, 0\}^T \, d\Omega \qquad (8)$$

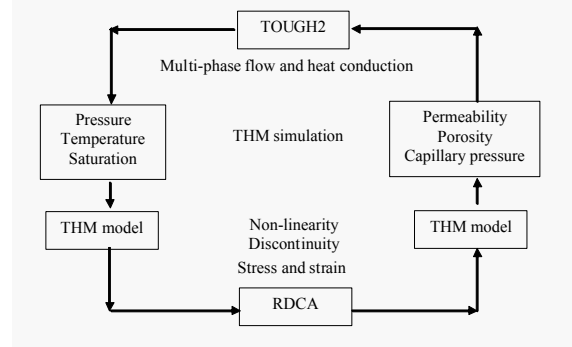where p is fluid pressure and B is strain-displacement matrix.

Figure 4. Schematic of linking TOUGH2 and EPCA for coupled thermo-hydro-mechanical (THM) simulations.
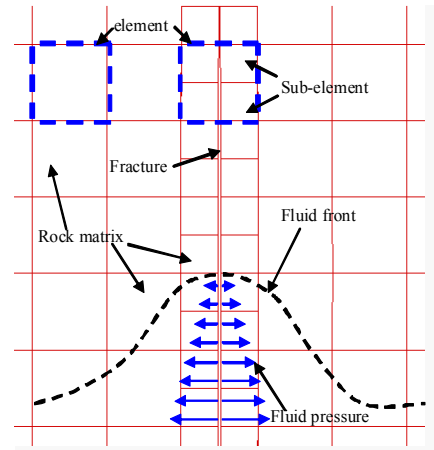

Figure 5. The mechanical state of rock mass induced by fluid flow

For elements that include crack surface or crack tip, the equivalent nodal force includes two parts. One is from the fluid pressure applied to the crack surface, as calculated by Eq. (1) and Eq. (2). The other is from the sub-elements, which are regarded as the rock matrix. Therefore, the contribution of sub-element on element equivalent nodal force can be calculated by Eq. (8), in which the matrix B is different from a normal element and the nodal force involves additional degrees of freedom.

Input parameters for the TOUGH simulation include grain density, porosity, permeability, thermal conductivity, specific heat, relative permeability and water retention curves, as well as hydraulic and thermal boundary conditions (e.g., fixed fluid pressure and temperature). Typical input parameters for the RDCA simulation include bulk density, elastic parameters (Young's modulus, Poisson's ratio), fracture-mechanics parameters (e.g., fracture toughness), as well as mechanical boundary conditions (e.g., fixed displacement or stress). We developed an external routine in which the THM model is included, linking TOUGH2 and RDCA. In this model, porosity, permeability, and capillary pressure are dependent on certain mechanical variables, such as mean stress, volumetric strain, or fracture aperture. For different applications, the THM model may be different.

NUMERICAL EXAMPLE RELATED TO GEOLOGIC CO$_2$ STORAGE

Problem description

We conducted a numerical simulation of hydromechanical changes during a deep underground injection of supercritical CO$_2$ in a hypothetical brine aquifer/caprock system, validating our TOUGH-RDCA simulator by comparing it with TOUGH-FLAC (Rutqvist and Tsang 2002) results.

In the modeling, CO$_2$ is injected at a constant rate over a 10-year period into a permeable injection zone at a depth of 1,300-1,500 m. The injection zone is overlain by a 100 m thick cap rock, located at 1,200-1,300 m, which in one of the studied cases is intersected by a vertical fault (Figure 6). The model description and parameters can be found in the work by Rutqvist and Tsang (2002). For the rock matrix, the constitutive relations of an isotropic linear poroelastic medium can be expressed in terms of the effective stress σ'_{ij} (positive for tension), strain ε_{ij} and temperature change ΔT as (Pan et al. 2009),

$$\sigma'_{ij} = 2G\left(\varepsilon_{ij} + \delta_{ij}\frac{v}{1-2v}\varepsilon_{kk}\right) - K'\alpha\Delta T\delta_{ij} \quad (9)$$

where $\sigma'_{ij} = \sigma_{ij} + \xi\bar{p}\delta_{ij}$ and σ_{ij} is the total stress (positive for tension), δ_{ij} is the Kronecker's del-

ta, $\xi(\leq 1)$ is a coefficient that depends on the compressibility of the constituents. Here, $\xi = 1$ is assumed. $\bar{p}$ is an average pore pressure defined as

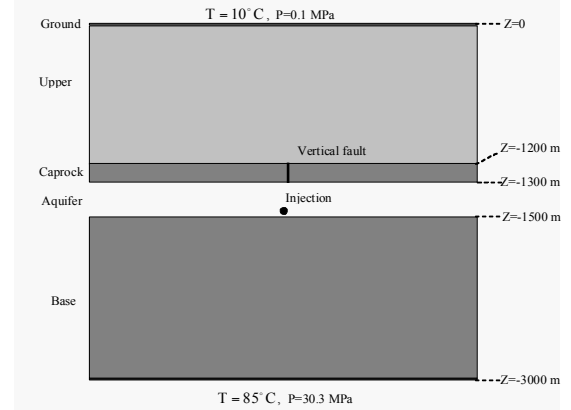$$\bar{p} = S_l p_l + (1 - S_l)p_g \quad (10)$$

Figure 6. Problem description

For rock fractures, the fluid pressure is applied on a fracture surface normal to the surface. If the shear stress on the fracture surface is not considered, the effective stress is expressed as

$$\sigma'_n = \sigma_n + \xi\bar{p} \quad (11)$$

Isotropic hydromechanical rock properties are represented by porosity-mean stress and permeability-porosity relationships. The porosity, φ, is related to the mean effective stress as (Rutqvist and Tsang 2002)

$$\varphi = (\varphi_0 - \varphi_r)\exp(5\times10^{-8}\times\sigma'_M) + \varphi_r \quad (12)$$

where ϕ_0 is porosity at zero stress, ϕ_r is residual porosity at high stress and the mean effective stress (in Pa) is defined from the stress components as

$$\sigma'_M = \frac{1}{3}(\sigma'_x + \sigma'_y + \sigma'_z) \quad (13)$$

Permeability is correlated to porosity according to the following exponential function:

$$k = k_0\exp[22.2(\varphi/\varphi_0 - 1)] \quad (14)$$

where k_0 is the zero stress permeability.

Homogeneous case

Figure 7 shows a comparison between different simulators with and without considering hydromechancial coupling. It is found that after 10 years' evolution, both TOUGH-FLAC and TOUGH-RDCA injection pressures are lower than that with TOUGH pure (uncoupled) hydraulic modeling. The TOUGH-RDCA modeling of injection pressure evolution has almost exactly the same results as those obtained with TOUGH-FLAC (maximum difference is 0.01 MPa in the 10th year), even though different models, i.e., 2D for RDCA and 3D for FLAC3D, are used.

Figure 8 shows a comparison of displacements at four points: (1) top of well at ground surface, (2) top of cap rock, (3) top of injection zone and (4) bottom of injection zone. The good agreement shows that TOUGH-RDCA displacement evolutions are consistent with that of TOUGH-FLAC. After 10 years of injection, the relative errors for these four points are 2.05%, 0.93%, 1.01% and 2.73%, respectively.

The small discrepancies between these two simulators may be induced by the sub-models used within RDCA and FLAC3D. The current RDCA system is based on a 2D formula that simplifies it to a plane strain problem, in which only σ_x, σ_y and τ_{xy} are independent variables, and σ_z given by $\sigma_z = v(\sigma_x + \sigma_y)$, where v is the Poisson's ratio. But in the FLAC3D model, all three components (σ_x, σ_y and σ_z) are independent variables, i.e., σ_z is not exactly equal to $v(\sigma_x + \sigma_y)$. Thus, although there are some differences between these two simulators, the results from TOUGH-RDCA are reasonable and acceptable for homogeneous cases.

The effect of fault in the caprock

We simulate a vertical fault (or fracture) within the cap rock to study its influence on cap-rock THM behavior. In RDCA, the fault is regarded as an internal boundary. By introducing the special displacement function, the discontinuity can be located arbitrarily in an element, which is divided into several sub-elements based on *partition of unity* concept. By doing so, the discontinuous boundary coincides with the edge of the sub-elements. In TOUGH2, the fracture is re-

garded as a porous medium. Initially, the fault has the same permeability as the cap rock. After fluid injection, it will open up and become more permeable than the surrounding cap rock (Figure 9). For the sake of simplicity, the permeability of a fracture element follows the same evolution rule as a matrix element.

Figure 10 shows the evolution of the CO_2 plume as a result of a constant rate injection. Already after 1 year injection, the CO_2 has penetrated into the fracture, but not yet up into the overlying aquifer. After 10 years' injection, the CO_2 plume has penetrated into the upper aquifer and spread laterally as well as upwards (by buoyancy) about 200 m.

Figure 11 and 12 show the evolution of fracture surface deformation. Figure 11 shows how the fracture opens, with the maximum opening at the center distance between the two crack tips, located just above and below the cap rock. Figure 12 shows the evolution of crack opening displacement (COD) at the inlet (at the bottom of the cap rock) and outlet (at the top of the cap rock). The COD increases more at the inlet because of the higher pressure changes compared to that at the outlet.
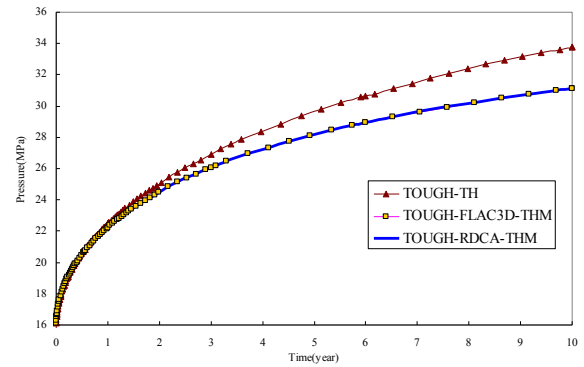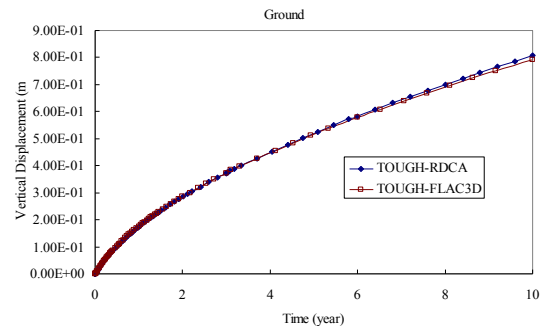

Figure 7. Injection pressure as a function of time with and without considering hydromechanical coupling effects—comparisons between different simulators.
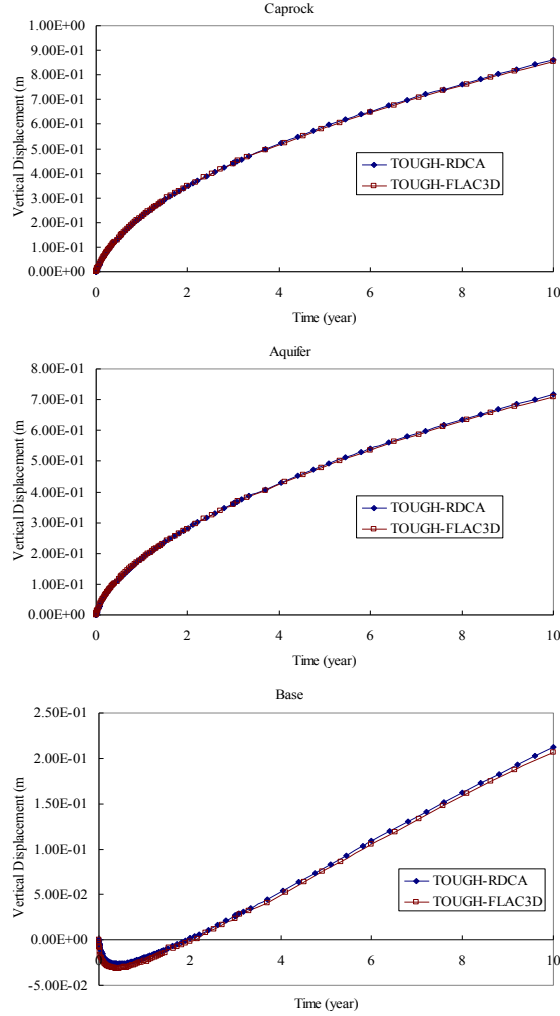
Figure 8. Vertical displacements during 10 years of CO2 injection on four points (i.e. (1) top of well at ground surface, (2) top of caprock, (3) top of injection zone and (4) bottom of injection zone) using different simulators.

Owing to the presence of the vertical fault (or fracture) in the rock mass, some of the reservoir pressure can be released. As a result, after 10 years of injection, the injection pressure decreases about 1.14 MPa compared with the result from homogeneous case (Figure 13).

By using a discontinuous method in RDCA, the detailed mechanical behaviors (e.g., fracture opening, close, or sliding) of fractures can be studied explicitly. This is different from the continuum method, in which the fracture zone is simulated as a porous medium that is more porous than the surrounding caprock and has a

much more sensitive HM relationship (Rutqvist and Tsang 2002). One of the disadvantages of this method is that the results are greatly dependent on element size. Higher precision requires a fine grid with small element sizes. RDCA completely overcomes this disadvantage through its special displacement functions to represent discontinuity. These functions include the Heaviside function for the discontinuous field along the length of the crack, and the near-tip function, which guarantees precision even though the numerical grid is relatively sparse.
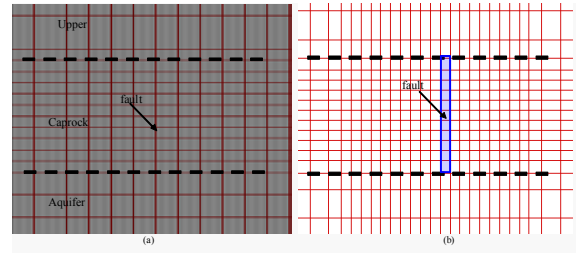

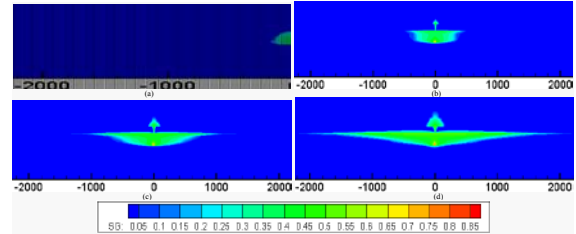Figure 9. Grids used in (a) RDCA and (b) TOUGH2

Figure 10. CO_2 saturation during active CO_2 injection at (a) 1 year; (b) 3 years; (c) 6 years, and (d) 10 years
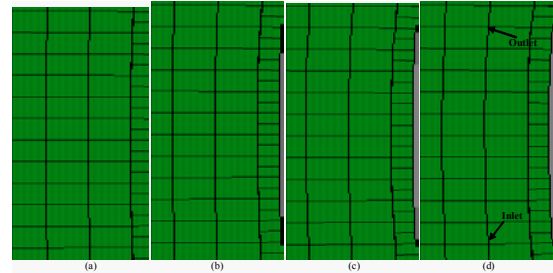

Figure 11. The fracture surface deformation (enlarge 10 times) during the injection of CO2. (a) 1 year; (b) 3 years; (c) 6 years and (d) 10 years.
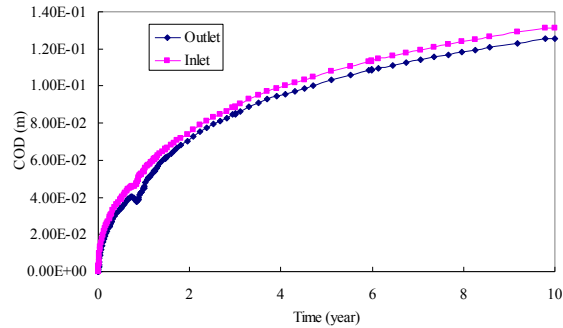
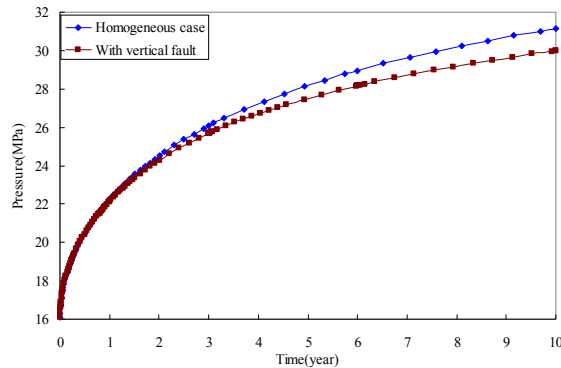Figure 12. The crack opening displacement evolution at inlet and outlet.

Figure 13. Injection pressure as a function of time with/without considering fault in cap rock.

CONCLUDING REMARKS

This paper demonstrates a numerical method that can simulate the nonlinearity and discontinuity of rock masses involving coupled multiphase nonisothermal fluid flow and geomechanics by linking the numerical codes TOUGH2 and RDCA. The preliminary results from numerical examples show that the TOUGH-RDCA simulator is capable of modeling discontinuous behavior in a rock mass under multiphase fluid flow conditions. More applications based on the developed simulators will be implemented and tested in the future, including fracture propagation.

ACKNOWLEDGMENTS

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